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On lattice Boltzmann scheme, finite volumes and boundary conditions

François Dubois ^{1 2} and Pierre Lallemand ³

¹ *Conservatoire National des Arts et Métiers, Paris, France.*

² *Numerical Analysis and Partial Differential Equations
Department of Mathematics, Paris Sud University, Orsay, France.*

³ *Applications Scientifiques du Calcul Intensif, Orsay, France.*

francois.dubois@math.u-psud.fr, pierre.lal@free.fr

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Abstract

We develop the idea that a natural link between Boltzmann schemes and finite volumes exists naturally: the conserved mass and momentum during the collision phase of the Boltzmann scheme induces general expressions for mass and momentum fluxes. We treat a unidimensional case and focus our development in two dimensions on possible flux boundary conditions. Several test cases show that a high level of accuracy can be achieved with this scheme.

Keywords : lattice Boltzmann scheme, boundary conditions, finite volume method.

1 Introduction

- The lattice Boltzmann scheme is a popular numerical method based on a kinetic approach for fluid dynamics ([HPP76] [DLF86] [FHP86] [MZ88] [HSB89] [DH92] [KR95] [LL00]). An exact propagation step in a lattice is followed by a local relaxation process. It has been very early recognized (see *e.g.* [BSV92]) that the lattice Boltzmann scheme is compatible with mass and momentum conservation. Similarly, classical conservation laws that lead

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to finite volume methods (see *e.g.* [Pa80], [GR96] or [DD05]) incorporate explicitly the evaluation of numerical fluxes associated with conserved physical quantities. In order to extend the lattice Boltzmann scheme to unstructured meshes, several authors [Ch98] [PXDC99] [UBS03] [USB04] start from the kinetic equations for the particle distribution and use control volumes “à la INRIA” [ADLV83] [Vi86], that is control volumes around the vertices of the triangulation.

- On the other hand, the treatment of boundary conditions with the help of boundary fluxes is natural with the so-called cell centered version of the finite volume method (see *e.g.* the classical monograph of Roache [Ro72] and our contributions [DL89] [Du01] in the strong nonlinear case). The incorporation of mass conservation *via* a zero mass flux on a solid boundary of the domain has been studied by D’Humières [DH01] and also developed in [vdS06] and [HHC06].

- In what follows, we start from a very general lattice Boltzmann scheme and propose to incorporate the fundamental conservations of mass and momentum in the framework of finite volumes. Then we propose to develop boundary conditions based on mass flux for the one-dimensional lattice Boltzmann scheme with three velocities. We extend the previous ideas for the so-called D2Q9 two-dimensional model. We extend also these ideas to the treatment of boundary conditions where the geometry of the control volumes has to be modified in order to take into account the physical geometry. Numerical simulations show the interest of our approach.

2 About the property of conservation

- We denote by \mathcal{L} a lattice, Δx a typical scale associated with this lattice, Δt a time step,

$$(1) \quad \lambda \equiv \frac{\Delta x}{\Delta t}$$

a typical speed of the problem, x a vertex of this lattice,

$$(2) \quad x_j \equiv x + \Delta t v_j, \quad 0 \leq j \leq J,$$

the set of neighbouring nodes around the vertex x . Note that the node defined by the relation (2) is a vertex of the lattice. We suppose that the family $(v_j)_{0 \leq j \leq J}$ of speeds is symmetric relative to the origin, as an example is shown in Figure 1.

$$(3) \quad \forall j \in \{0, \dots, J\}, \quad \exists! \sigma(j) \in \{0, \dots, J\}, \quad v_j + v_{\sigma(j)} = 0.$$

We remark the clear property of involution:

$$(4) \quad \sigma(\sigma(j)) = j, \quad 0 \leq j \leq J.$$

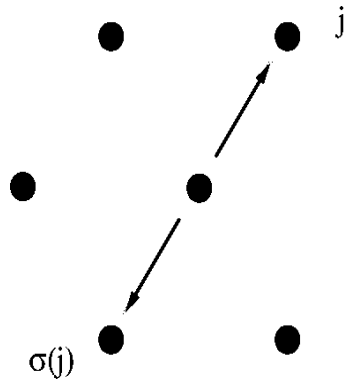


Figure 1. Central symmetry hypothesis

- Let $f_j(x, t)$ be a distribution of particles on the lattice \mathcal{L} at the vertex x and discrete time t . We recall [FHHLPR87] (see also [CD98] or [LL00]) that the discrete dynamics of this distribution on the lattice \mathcal{L} is given by a collision step followed by a free advection displacement between two nodes. We assume that the density

$$(5) \quad \rho \equiv \sum_j f_j$$

and the momentum

$$(6) \quad q \equiv \sum_j v_j f_j$$

are conserved during the collision step and we denote by $f_j^*(x, t)$ the distribution after this step:

$$(7) \quad \rho \equiv \sum_j f_j = \sum_j f_j^* \equiv \rho^*,$$

$$(8) \quad q \equiv \sum_j v_j f_j = \sum_j v_j f_j^* \equiv q^*.$$

Then the dynamics of the lattice Boltzmann scheme takes the simple form [Du08]

$$(9) \quad f_j(x, t + \Delta t) = f_j^*(x - v_j \Delta t, t), \quad x \in \mathcal{L}, \quad 0 \leq j \leq J.$$

We restrict in what follows to numerical physics that conserve mass and momentum. The incorporation of conservation of energy is also possible and we refer to [LL03] which discusses various attempts to include energy conservation. Note that the state of the art concerning the collision step $f \rightarrow f^*$ is due to [DH92] with the so-called ‘‘multiple relaxation time’’ Boltzmann scheme. Remark that in all this contribution the choice of the relaxation model has no influence on our methodology.

• **Proposition 1. Conservation property.**

We have the following relations concerning the temporal evolution of conserved momenta

$$(10) \quad \rho(x, t + \Delta t) - \rho(x, t) + \sum_j (f_j^*(x, t) - f_{\sigma(j)}^*(x_j, t)) = 0$$

$$(11) \quad q(x, t + \Delta t) - q(x, t) + \sum_j v_j (f_j^*(x, t) + f_{\sigma(j)}^*(x_j, t)) = 0.$$

Proof of Proposition 1.

We have from the dynamics (9) by summation over the index j

$$\begin{aligned} \rho(x, t + \Delta t) &= \sum_j f_j^*(x - v_j \Delta t, t) = \sum_j f_{\sigma(j)}^*(x - v_{\sigma(j)} \Delta t, t) = \\ &= \sum_j f_{\sigma(j)}^*(x + v_j \Delta t, t) = \sum_j f_{\sigma(j)}^*(x_j, t) \end{aligned}$$

and the relation (10) is established due to (7). In an analogous way, we have for the momentum:

$$\begin{aligned} q(x, t + \Delta t) &= \sum_j v_j f_j^*(x - v_j \Delta t, t) = \sum_j v_{\sigma(j)} f_{\sigma(j)}^*(x - v_{\sigma(j)} \Delta t, t) = \\ &= - \sum_j v_j f_{\sigma(j)}^*(x + v_j \Delta t, t) = - \sum_j v_j f_{\sigma(j)}^*(x_j, t) \end{aligned}$$

and the relation (11) follows from (8). \square

- We suppose now that we can introduce a cell $K(x)$ around the vertex x such that its boundary $\partial K(x)$ is composed by J edges $a_j(x)$ separating the nodes x and x_j :

$$(12) \quad \partial K(x) = \bigcup_{j>0} a_j(x),$$

with edges $a_j(x)$ such that

$$(13) \quad a_j(x) = \partial K(x) \cap \partial K(x_j) = a_{\sigma(j)}(x_j).$$

We denote by $|K(x)|$ and $|a_j(x)|$ the measures of $K(x)$ and $a_j(x)$ respectively. Then the conservation of mass and momentum takes the discrete form

$$(14) \quad \frac{1}{\Delta t} \left[\rho(x, t + \Delta t) - \rho(x, t) \right] + \frac{1}{|K(x)|} \sum_j |a_j(x)| \psi_j(x) = 0,$$

$$(15) \quad \frac{1}{\Delta t} \left[q(x, t + \Delta t) - q(x, t) \right] + \frac{1}{|K(x)|} \sum_j |a_j(x)| \zeta_j(x) = 0.$$

- **Proposition 2. An algebraic expression for general fluxes.**

We suppose that the lattice Boltzmann scheme (7) (8) (9) satisfies the above hypotheses (12) and (13) and that the control volumes $K(x)$ and $K(x_j)$ have the same measure:

$$(16) \quad |K(x)| = |K(x_j)|, \quad 1 \leq j \leq J.$$

We define the mass flux ψ_j and the momentum flux ζ_j with the following expressions:

$$(17) \quad \psi_j(x) = \frac{|K(x)|}{\Delta t |a_j(x)|} (f_j^*(x) - f_{\sigma(j)}^*(x_j)),$$

$$(18) \quad \zeta_j(x) = \frac{|K(x)|}{\Delta t |a_j(x)|} v_j (f_j^*(x) + f_{\sigma(j)}^*(x_j)).$$

Then the quantities defined in (17) and (18) are so-called “conservative fluxes” in the following sense:

$$(19) \quad \psi_j(x) + \psi_{\sigma(j)}(x_j) = 0$$

$$(20) \quad \zeta_j(x) + \zeta_{\sigma(j)}(x_j) = 0.$$

with the vertex x_j defined in (2).

Proof of Proposition 2.

The first part of the proposition is simply obtained by considering that (10) [respectively (11)] and (14) [respectively (15)] define identically the same evolution equation. Then we have for the conservation property of mass:

$$\begin{aligned} \psi_j(x) + \psi_{\sigma(j)}(x_j) &= \\ &= \frac{|K(x)|}{\Delta t |a_j(x)|} (f_j^*(x) - f_{\sigma(j)}^*(x_j)) + \frac{|K(x_j)|}{\Delta t |a_{\sigma(j)}(x_j)|} (f_{\sigma(j)}^*(x_j) - f_{\sigma(\sigma(j))}^*(x)) \\ &= \frac{|K(x)|}{\Delta t |a_j(x)|} (f_j^*(x) - f_{\sigma(j)}^*(x_j)) + \frac{|K(x)|}{\Delta t |a_j(x)|} (f_{\sigma(j)}^*(x_j) - f_j^*(x)) \\ &\hspace{15em} \text{due to (13), (16) and (4).} \\ &= 0. \end{aligned}$$

Analogously for the momentum:

$$\begin{aligned} \zeta_j(x) + \zeta_{\sigma(j)}(x_j) &= \frac{|K(x)|}{\Delta t |a_j(x)|} v_j (f_j^*(x) + f_{\sigma(j)}^*(x_j)) + \\ &\quad + \frac{|K(x_j)|}{\Delta t |a_{\sigma(j)}(x_j)|} v_{\sigma(j)} (f_{\sigma(j)}^*(x_j) + f_{\sigma(\sigma(j))}^*(x)) \\ &= \frac{|K(x)|}{\Delta t |a_j(x)|} v_j (f_j^*(x) + f_{\sigma(j)}^*(x_j)) - \frac{|K(x_j)|}{\Delta t |a_{\sigma(j)}(x_j)|} v_j (f_{\sigma(j)}^*(x_j) + f_j^*(x)) \\ &\hspace{15em} \text{due to (3) and the previous arguments} \\ &= 0 \end{aligned}$$

and the property is established. \square

- This remark makes a clear link between the lattice Boltzmann scheme and the finite volume method [Pa80]. Note that the hypothesis (16) can be not satisfied for the boundary cells as we will see in the following. In that case, we adapt the definition of the flux in order to enforce the conservation conditions (19) and (20).

3 Flux boundary condition for the D1Q3 model

- In the particular case of D1Q3 model [QHL92] (see also all algebraic details in [Du07]), each vertex x of the lattice has two neighbours $x_- \equiv x - \Delta x$ and $x_+ \equiv x + \Delta x$. Then the number of particles with velocity equal to $-\lambda$ [respectively $0, +\lambda$] is denoted by f^- [respectively f^0 and f^+]. The bijection σ introduced in (3) is given simply according to

$$(21) \quad \sigma(0) = 0, \quad \sigma(+)= -, \quad \sigma(-) = +.$$

Moreover, there is a geometrical and topological evidence that a cell $K(x)$ can be constructed around the vertex x :

$$(22) \quad K(x) =]x - \frac{\Delta x}{2}, x + \frac{\Delta x}{2}[.$$

as illustrated in Figure 2.

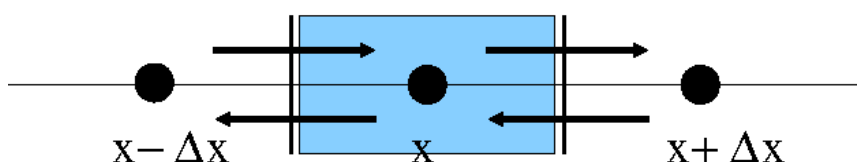


Figure 2. Uni-dimensional cell $K(x)$ around the vertex x .

We observe that

$$(23) \quad |K(x)| = \Delta x.$$

The boundary $\partial K(x)$ is composed by 2 “point-like edges” $a_-(x)$ and $a_+(x)$ such that

$$(24) \quad |a_{\pm}(x)| = 1.$$

• **Proposition 3. Fluxes for the D1Q3 model.**

In one space dimension (D1Q3 model) the lattice Boltzmann scheme is exactly a finite volume method. The mass flux ψ and momentum flux ζ are given by the expressions (17) and (18) that take in this particular case the form:

$$(25) \quad \psi_j(x) = \lambda (f_j^*(x) - f_{\sigma(j)}^*(x_j)), \quad j = -, 0, +.$$

$$(26) \quad \zeta_j(x) = \lambda v_j (f_j^*(x) + f_{\sigma(j)}^*(x_j)), \quad j = -, 0, +.$$

Proof of Proposition 3.

We have simply the relations (10) and (11) that can be re-written introducing (1) and (23):

$$\begin{aligned} \frac{1}{\Delta t} (\rho(x, t + \Delta t) - \rho(x, t)) + \frac{1}{\Delta x} \sum_j \lambda (f_j^*(x, t) - f_{\sigma(j)}^*(x_j, t)) &= 0 \\ \frac{1}{\Delta t} (q(x, t + \Delta t) - q(x, t)) + \frac{1}{\Delta x} \sum_j \lambda v_j (f_j^*(x, t) + f_{\sigma(j)}^*(x_j, t)) &= 0 \end{aligned}$$

id est a vectorial discrete conservation law of the form

$$\frac{1}{\Delta t} [W(x, t + \Delta t) - W(x, t)] + \frac{1}{|K(x)|} \int_{\partial K} \Phi \cdot n \, d\gamma = 0$$

with a vector W composed by density ρ and momentum q . Then the relations (25) and (26) are clear. \square

• We remark also that we generalize in what follows the terminology “finite volume method”. According *e.g.* to the classical reference [GR96], the definition of a flux requires *a priori* fluxes to be functions of just the conserved variables. Here mass flux and momentum flux cannot be expressed in terms of the only conserved variables (mass and momentum densities) but are in contrary functions of all particle distributions f .

• We study now the problem of defining a boundary condition for our D1Q3 Boltzmann model [GA94], [GH03]. We focus on the particular case of the presence of a wall at one of the extremities. We suppose that x is a vertex of the lattice internal to the domain under study and that its right neighbour x_+ is external to the computational domain. Moreover, the geometric position

x_w of the wall is not supposed to be exactly between x and x_+ but at a certain fraction ξ :

$$(27) \quad x_w = x + \xi \Delta x, \quad 0 < \xi < 1.$$

Note that the particular case $\xi = \frac{1}{2}$ corresponds to a position of the wall at equal distance between the “last” vertex inside the domain and the “first” vertex outside the computational domain.

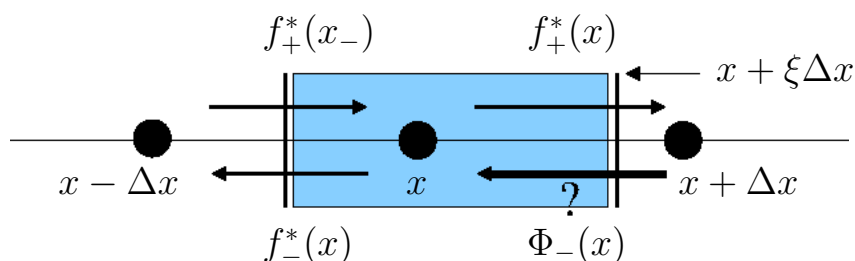


Figure 3. Numerical boundary condition for the D1Q3 model.

- Assuming the computational domain has nontrivial extent, we suppose that both vertices x and x_- are located inside the computational domain. At a certain discrete time t , we have at our disposal the particle transfer $f_0^*(x)$ of null velocity at the vertex x , the particle transfer $f_-^*(x)$ of speed $-\lambda$ from vertex x to the point x_- , the particle transfer $f_+^*(x_-)$ of speed λ from point x_- towards vertex x . We denote by $\Phi_-(x)$ (instead of $f_-^*(x_+)$) the unknown particle transfer of speed $-\lambda$ coming from the “ghost” vertex x_+ towards the vertex x . This quantity has to be determined by the so-called “numerical boundary scheme”. All the above notations are illustrated in Figure 3.

- At a boundary vertex x , we modify the construction of the control volume $K(x)$ and introduce a natural finite volume defined at the left by the intermediate vertex $x - \frac{\Delta x}{2}$ and on the right by the boundary vertex x_w . Such a control volume satisfies

$$(28) \quad |K(x)| = \left(\xi + \frac{1}{2} \right) \Delta x.$$

We observe that $|K(x)|$ is equal to Δx only when $\xi = \frac{1}{2}$.

• At a boundary, a good numerical methodology is to impose a flux (see *e.g.* [DL89]). This approach is natural with a finite volume methodology. At the solid boundary located at $x = x_w$, the physical impermeability condition leads to a **zero mass flux** $\psi_+(x)$:

$$(29) \quad \psi_+(x) = 0.$$

If we evaluate this mass flux according to the relation (25), we obtain in this particular case: $\psi_+(x) = \lambda(f_+^*(x) - \Phi_-(x))$ and due to (29), we obtain in this manner the so-called “bounce-back” boundary condition:

$$(30) \quad \Phi_-(x) = f_+^*(x).$$

Other interpolation schemes have been proposed by several authors, for example [MLS99] [BFL01].

• **Scheme 1. Flux boundary condition for the D1Q3 model.**

Our finite volume boundary condition consists in considering Figure 3 as a finite control box $K(x)$ around vertex x with a particular shape imposed by the geometry of the problem. The boundary is located at a distance $\xi\Delta x$ from the vertex x . We propose to use the following formula for the unknown input particle number:

$$(31) \quad \Phi_-(x) = f_+^*(x) + \frac{\xi - \frac{1}{2}}{\xi + \frac{1}{2}} \left(f_-^*(x) - f_+^*(x_-) \right).$$

Construction of Scheme 1.

We make a mass balance in a mesh $K(x)$ of measure given by (28) that takes into account the boundary. In order to enforce the conservation property, the left mass flux $\psi_-(x)$ in the direction $x \rightarrow x - \Delta x$ is *a priori* still given according to the relation (25)

$$(32) \quad \psi_-(x) = \lambda(f_-^*(x) - f_+^*(x - \Delta x))$$

and the right mass flux $\psi_+(x)$ is null (see (29)). We then write the time evolution of the scheme in two ways. First, we have the general mass conservation (10) of a Boltzmann scheme that takes here the form:

$$(33) \quad \rho(x, t + \Delta t) - \rho(x, t) + (f_+^*(x) - \Phi_-(x)) + (f_-^*(x) - f_+^*(x - \Delta x)) = 0.$$

Second, we have the mass conservation (19) inside the volume $K(x)$:

$$(34) \quad \frac{1}{\Delta t} (\rho(x, t + \Delta t) - \rho(x, t)) + \frac{1}{|K(x)|} [\psi_+(x) + \psi_-(x)] = 0.$$

We use (28), (32) and the physical condition (29) in order to eliminate the term $(\rho(x, t + \Delta t) - \rho(x, t))$ between the relations (33) and (34). We obtain:

$$(f_+^*(x) - \Phi_-(x)) + (f_-^*(x) - f_+^*(x - \Delta x)) = \frac{1}{\xi + \frac{1}{2}} (f_-^*(x) - f_+^*(x - \Delta x))$$

and we extract $\Phi_-(x)$ from the above expression. Then relation (31) is established and the scheme is constructed. \square

- The numerical boundary scheme (31) has been derived as a consequence of the mass conservation and a precise treatment of the no-penetration boundary condition (29). This constraint of mass conservation at the boundary has been studied by [NCG95]. Note that with their own treatment [GH03] of the boundary condition, Ginzburg and D'Humières have proposed a boundary scheme very close to (31) that conserves mass in one space dimension [DH01] [DH06].

- **Proposition 4. Linearity of the mass flux.**

The relation (31) is what is obtained if we suppose that the mass flux defined in the x direction by the relations

$$(35) \quad \psi\left(-\frac{\Delta x}{2}\right) = \lambda(f_+^*(x - \Delta x) - f_-^*(x))$$

$$(36) \quad \psi\left(\frac{\Delta x}{2}\right) = \lambda(f_+^*(x) - \Phi_-(x))$$

$$(37) \quad \psi(\xi \Delta x) = 0$$

at respective positions $-\frac{\Delta x}{2}$, $\frac{\Delta x}{2}$ and $\xi \Delta x$ at the boundary is **linear**.

Proof of Proposition 4.

We remark first that $\psi\left(-\frac{\Delta x}{2}\right) = -\psi_-(x)$ (defined in (32)) due to the choice of the direction to measure this mass flux. The condition of linearity for the function defined by the relations (35), (36) and (37) can be expressed under the form

$$\frac{0 - \lambda(f_+^*(x - \Delta x) - f_-^*(x))}{\xi \Delta x - \left(-\frac{\Delta x}{2}\right)} = \frac{0 - \lambda(f_+^*(x) - \Phi_-(x))}{\xi \Delta x - \frac{\Delta x}{2}}$$

that is

$$\frac{f_+^*(x - \Delta x) - f_-^*(x)}{\xi + \frac{1}{2}} = \frac{f_+^*(x) - \Phi_-(x)}{\xi - \frac{1}{2}}$$

and the last relation corresponds exactly to (31). □

- **Uni-dimensional acoustic wave.**

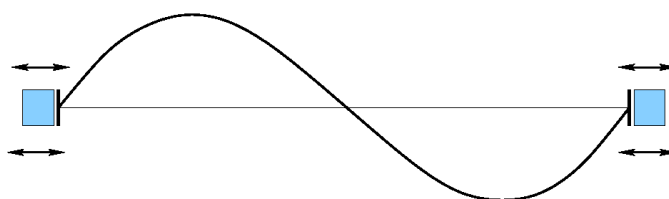


Figure 4. Uni-dimensional acoustic wave.

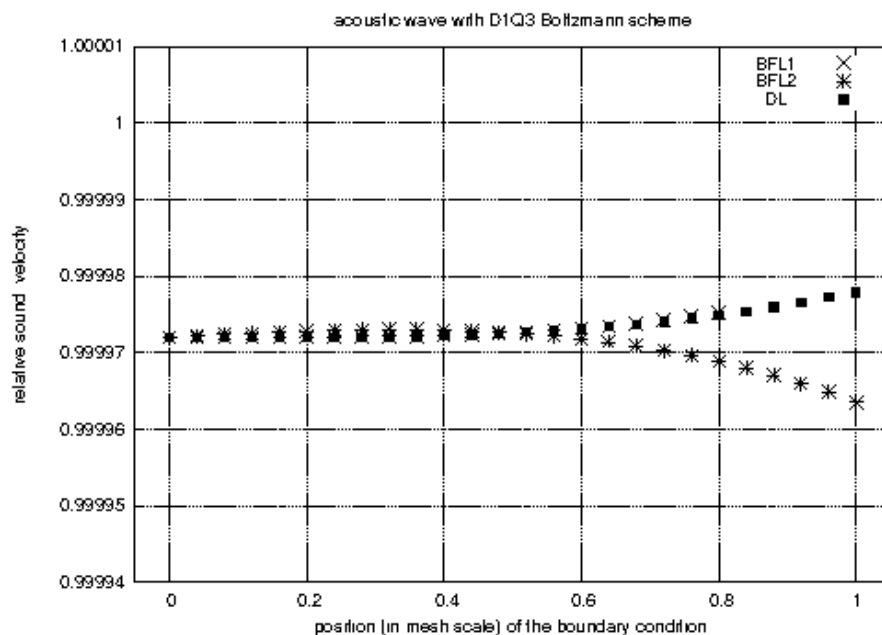


Figure 5. Relative sound velocity with D1Q3 lattice Boltzmann scheme for various schemes and a mesh of 100 points.

- We have tested the above idea in the case of an acoustic wave in a tube closed at the two extremities. We are able to produce a variation of the

boundary condition location by a fraction ξ of the mesh Δx (see Figure 4). We determine the eigenvalues of the operator that corresponds to one time step of the LB algorithm, using the ARPACK [LSY96] software package. For the lowest mode with effective wave vector

$$(38) \quad k = \frac{\pi}{(N - 1 + 2\xi)\Delta x}$$

this leads to $-\gamma_r + i\gamma_i$ from which we determine an effective speed of sound

$$(39) \quad c_{\text{rel}} = \frac{\gamma_i}{c_s k}$$

if there are N lattice points between the boundaries. We introduce similarly the effective relative attenuation

$$(40) \quad a_{\text{rel}} = \frac{\gamma_r}{\frac{1}{2}\nu_\ell k^2}$$

with ν_ℓ the longitudinal kinematic viscosity [LL59]. The relative value of sound velocity is displayed in Figure 5 and Table 1. The results of our scheme are comparable with those of Bouzidi *al.* [BFL01] when using linear extrapolation. After a simple exploitation of Table 1 with least squares, the error for sound velocity with bounce-back scheme is proportional to $\frac{1}{N}$ whereas it is proportional to $\frac{1}{N^2}$ for both versions of the Bouzidi scheme and our scheme.

	100 points	200 points	300 points
bounce-back	9.97231×10^{-3}	4.99309×10^{-3}	3.33025×10^{-3}
BFL1	2.797×10^{-5}	6.94×10^{-6}	3.09×10^{-6}
BFL2	3.645×10^{-5}	8.02×10^{-6}	3.41×10^{-6}
DL	2.803×10^{-5}	6.95×10^{-6}	3.09×10^{-6}

Table 1. Largest discrepancy of the relative sound velocity with D1Q3 lattice Boltzmann scheme for various boundary schemes and meshes.

- We give in Figure 6 and Table 2 various results for the effective attenuation a_{rel} . Our method is spectacularly better than the linear extrapolation case (“BFL1”) and comparable with the quadratic interpolation scheme

(“BFL2”) of the previous authors [BFL01] when the boundary is not located exactly half-way between two mesh points and equivalent to the previous one in this particular geometric case. After an elementary exploitation of Table 2, bounce-back and linear extrapolation version of Bouzidi scheme give an error for attenuation of the first eigenmode proportional to $\frac{1}{N}$. This error for attenuation is proportional to $\frac{1}{N^2}$ with quadratic extrapolation version of Bouzidi scheme and proportional to $\frac{1}{N^3}$ with the present scheme.

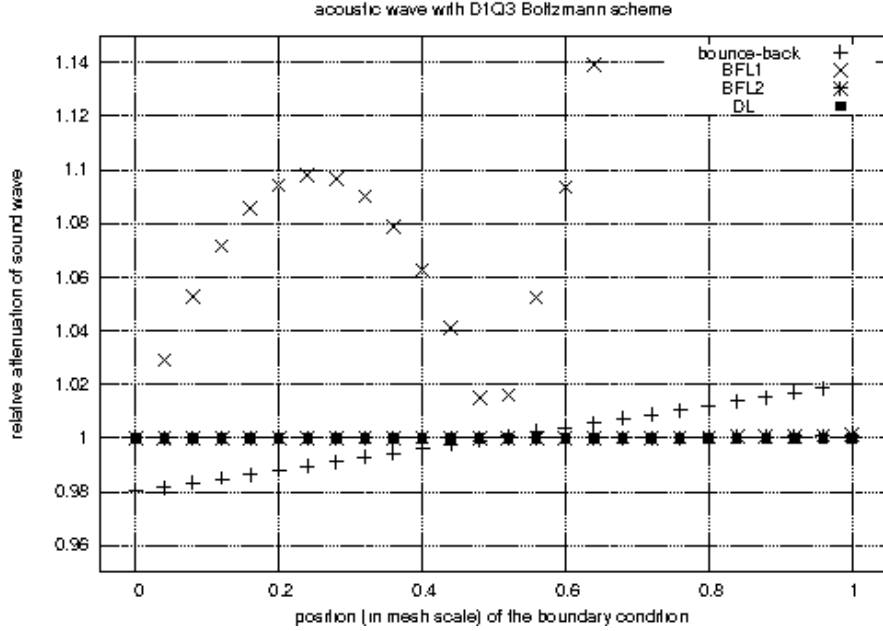


Figure 6. Relative attenuation of an acoustic wave for various numerical boundary Boltzmann schemes and a mesh of 100 points.

	100 points	200 points	300 points
bounce-back	2.009999×10^{-2}	1.002496×10^{-2}	6.67772×10^{-3}
BFL1	0.77150864	0.38796054	0.25910648
BFL2	1.10138×10^{-3}	1.3972×10^{-4}	4.157×10^{-5}
DL	9.57×10^{-6}	1.17×10^{-6}	3.1×10^{-7}

Table 2. Largest discrepancy of the relative attenuation of an acoustic wave for various numerical boundary Boltzmann schemes and meshes.

4 Finite volumes for the D2Q9 model

• We have two formulae for the time evolution of the conserved momenta: the evolution of mass (10) and momentum (11) that comes from the general properties of a lattice Boltzmann scheme and the finite volumes framework (14) (15). For the case of the two dimensional model D2Q9 (defined *e.g.* in [QHL92]), we set two natural questions: (i) Where is (geometrically !!) the finite volume $K(x)$? (ii) What are the possible formulae for the mass flux ψ_j and the momentum flux ζ_j ? To our knowledge, there is no satisfying answer to the above questions ! We suggest here to use **two** different control finite volumes K_{\parallel} and K_{\times} defined in Figure 7 and essentially to neglect the internal dynamics between the two control volumes during the relaxation step.

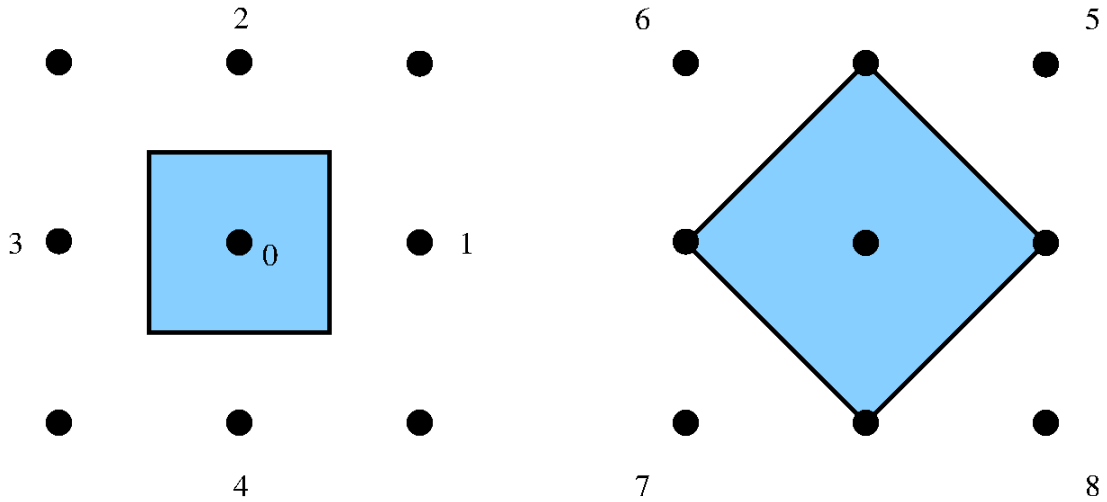


Figure 7. Control finite volumes K_{\parallel} and K_{\times} for the two-dimensional D2Q9 lattice Boltzmann scheme.

• We look carefully at Figure 7 and we observe that

$$(41) \quad |K_{\parallel}| = \Delta x^2, \quad |K_{\times}| = 2 \Delta x^2.$$

Moreover the boundary ∂K_{\parallel} [respectively ∂K_{\times}] is composed by the four edges a_j for $j = 1$ to 4 [respectively $j = 5$ to 8] and we have

$$(42) \quad |a_j| = \Delta x, \quad j = 1, 2, 3, 4, \quad |a_j| = \sqrt{2} \Delta x, \quad j = 5, 6, 7, 8.$$

- We introduce the partial densities $\rho_{\parallel}(x, t)$, $\rho_{\times}(x, t)$ and the partial momenta $q_{\parallel}(x, t)$, $q_{\times}(x, t)$ according to

$$(43) \quad \rho_{\parallel}(x, t) = \sum_{j=0}^4 f_j(x, t), \quad \rho_{\times}(x, t) = \sum_{j=5}^8 f_j(x, t)$$

$$(44) \quad q_{\parallel}(x, t) = \sum_{j=0}^4 v_j f_j(x, t), \quad q_{\times}(x, t) = \sum_{j=5}^8 v_j f_j(x, t)$$

and the analogous quantities $\rho_{\parallel}^*(x, t)$, $\rho_{\times}^*(x, t)$, $q_{\parallel}^*(x, t)$, $q_{\times}^*(x, t)$ by replacing f by f^* after collisions in the relations (43) and (44). We introduce also the defect of conservation of the partial momenta:

$$(45) \quad \Delta\rho \equiv \rho_{\parallel}^*(x, t) - \rho_{\parallel}(x, t), \quad \Delta q \equiv q_{\parallel}^*(x, t) - q_{\parallel}(x, t).$$

- **Proposition 5. Internal defect of conservation.**

With the above definitions, we have

$$(46) \quad \rho_{\parallel}(x, t + \Delta t) - \rho_{\parallel}(x, t) + \sum_{j=0}^4 (f_j^*(x, t) - f_{\sigma(j)}^*(x_j, t)) = \Delta\rho$$

$$(47) \quad \rho_{\times}(x, t + \Delta t) - \rho_{\times}(x, t) + \sum_{j=5}^8 (f_j^*(x, t) - f_{\sigma(j)}^*(x_j, t)) = -\Delta\rho$$

$$(48) \quad q_{\parallel}(x, t + \Delta t) - q_{\parallel}(x, t) + \sum_{j=0}^4 v_j (f_j^*(x, t) + f_{\sigma(j)}^*(x_j, t)) = \Delta q$$

$$(49) \quad q_{\times}(x, t + \Delta t) - q_{\times}(x, t) + \sum_{j=5}^8 v_j (f_j^*(x, t) + f_{\sigma(j)}^*(x_j, t)) = -\Delta q.$$

Proof of Proposition 5.

It is a direct consequence of the definitions (43), (44), (45) and of the microscopic iteration of the scheme (9). To fix the ideas, we detail the proof of (46):

$$\rho_{\parallel}(x, t + \Delta t) - \rho_{\parallel}(x, t) = \sum_{j=0}^4 f_j^*(x - v_j \Delta t, t) - \rho_{\parallel}^*(x, t) + \Delta\rho$$

$$\begin{aligned}
&= \sum_{j=0}^4 f_{\sigma(j)}^*(x - v_j \Delta t, t) - \sum_{j=0}^4 f_j^*(x, t) + \Delta \rho \\
&= - \sum_{j=0}^4 (f_j^*(x, t) - f_{\sigma(j)}^*(x - v_j \Delta t, t)) + \Delta \rho. \quad \square
\end{aligned}$$

• In what follows, we neglect the difference between $\rho_{\parallel}(x, t + \Delta t) - \rho_{\parallel}(x, t)$ and $\rho_{\parallel}(x, t + \Delta t) - \rho_{\parallel}^*(x, t)$ when we suppose that $\Delta \rho$ is equal to zero. In other terms, the partial masses ρ_{\parallel} and ρ_{\times} are supposed to be conserved during the collision process. Of course, we make the same hypothesis for the momentum and the differences $q_{\parallel}(x, t + \Delta t) - q_{\parallel}(x, t)$ and $q_{\parallel}(x, t + \Delta t) - q_{\parallel}^*(x, t)$ are neglected when Δq is supposed to be negligible. We have the following proposition that uses explicitly the less natural increment $\rho_{\parallel}(x, t + \Delta t) - \rho_{\parallel}^*(x, t)$ and associated.

• **Proposition 6. Partial numerical fluxes.**

We have the following expressions for the time evolution

$$(50) \quad \frac{1}{\Delta t} \left[\rho_{\parallel}(x, t + \Delta t) - \rho_{\parallel}^*(x, t) \right] + \frac{1}{|K_{\parallel}|} \sum_{j=0}^4 |a_j| \psi_j(x) = 0,$$

$$(51) \quad \frac{1}{\Delta t} \left[\rho_{\times}(x, t + \Delta t) - \rho_{\times}^*(x, t) \right] + \frac{1}{|K_{\times}|} \sum_{j=5}^8 |a_j| \psi_j(x) = 0,$$

$$(52) \quad \frac{1}{\Delta t} \left[q_{\parallel}(x, t + \Delta t) - q_{\parallel}^*(x, t) \right] + \frac{1}{|K_{\parallel}|} \sum_{j=0}^4 |a_j| \zeta_j(x) = 0,$$

$$(53) \quad \frac{1}{\Delta t} \left[q_{\times}(x, t + \Delta t) - q_{\times}^*(x, t) \right] + \frac{1}{|K_{\times}|} \sum_{j=5}^8 |a_j| \zeta_j(x) = 0,$$

with “mass fluxes” $\psi_j(x)$ given by

$$(54) \quad \psi_j(x) = \lambda (f_j^*(x, t) - f_{\sigma(j)}^*(x_j, t)), \quad 0 \leq j \leq 4$$

$$(55) \quad \psi_j(x) = \lambda \sqrt{2} (f_j^*(x, t) - f_{\sigma(j)}^*(x_j, t)), \quad 5 \leq j \leq 8$$

and “momentum fluxes” $\zeta_j(x)$ by

$$(56) \quad \zeta_j(x) = \lambda v_j (f_j^*(x, t) + f_{\sigma(j)}^*(x_j, t)), \quad 0 \leq j \leq 4$$

$$(57) \quad \zeta_j = \lambda v_j \sqrt{2} (f_j^*(x, t) + f_{\sigma(j)}^*(x_j, t)), \quad 5 \leq j \leq 8.$$

Proof of Proposition 6.

We simply make the partial sums from the fundamental evolution relation (9) and we get by introducing the space scale Δx , the time scale Δt , and their ratio λ :

$$\begin{aligned} \frac{1}{\Delta t} (\rho_{\parallel}(x, t + \Delta t) - \rho_{\parallel}^*(x, t)) + \frac{1}{\Delta x} \sum_{j=0}^4 \lambda (f_j^*(x, t) - f_{\sigma(j)}^*(x_j, t)) &= 0 \\ \frac{1}{\Delta t} (\rho_{\times}(x, t + \Delta t) - \rho_{\times}^*(x, t)) + \frac{1}{\Delta x} \sum_{j=5}^8 \lambda (f_j^*(x, t) - f_{\sigma(j)}^*(x_j, t)) &= 0 \\ \frac{1}{\Delta t} (q_{\parallel}(x, t + \Delta t) - q_{\parallel}^*(x, t)) + \frac{1}{\Delta x} \sum_{j=0}^4 \lambda v_j (f_j^*(x, t) + f_{\sigma(j)}^*(x_j, t)) &= 0 \\ \frac{1}{\Delta t} (q_{\times}(x, t + \Delta t) - q_{\times}^*(x, t)) + \frac{1}{\Delta x} \sum_{j=5}^8 \lambda v_j (f_j^*(x, t) + f_{\sigma(j)}^*(x_j, t)) &= 0. \end{aligned}$$

We replace in the above expressions the space scale Δx , by the correct expression as function of (41) and (42):

$$\begin{aligned} \frac{1}{\Delta t} (\rho_{\parallel}(x, t + \Delta t) - \rho_{\parallel}^*(x, t)) + \sum_{j=0}^4 \frac{|a_j|}{|K_{\parallel}|} \lambda (f_j^*(x, t) - f_{\sigma(j)}^*(x_j, t)) &= 0 \\ \frac{1}{\Delta t} (\rho_{\times}(x, t + \Delta t) - \rho_{\times}^*(x, t)) + \sum_{j=5}^8 \frac{|a_j|}{|K_{\times}|} \lambda \sqrt{2} (f_j^*(x, t) - f_{\sigma(j)}^*(x_j, t)) &= 0 \\ \frac{1}{\Delta t} (q_{\parallel}(x, t + \Delta t) - q_{\parallel}^*(x, t)) + \sum_{j=0}^4 \frac{|a_j|}{|K_{\parallel}|} \lambda v_j (f_j^*(x, t) + f_{\sigma(j)}^*(x_j, t)) &= 0 \\ \frac{1}{\Delta t} (q_{\times}(x, t + \Delta t) - q_{\times}^*(x, t)) + \sum_{j=5}^8 \frac{|a_j|}{|K_{\times}|} \lambda \sqrt{2} v_j (f_j^*(x, t) + f_{\sigma(j)}^*(x_j, t)) &= 0. \end{aligned}$$

We have clearly an exact equivalence between the four above expressions with the relations (50), (51), (52) and (53) if we make the choices (54), (55), (56) and (57) for the fluxes. \square

- We remark that we have proposed to cut the density (and the momentum) into two parts ρ_{\parallel} and ρ_{\times} : $\rho \equiv \rho_{\parallel} + \rho_{\times}$ and we have also $\rho^* \equiv \rho_{\parallel}^* + \rho_{\times}^*$ but keep in memory that we do not have a conservation law for the partial densities: $\rho_{\parallel}^* \neq \rho_{\parallel}$ and $\rho_{\times}^* \neq \rho_{\times}$ *a priori* even if $\rho^* \equiv \rho$. We have a similar remark for the momentum: $q_{\parallel}^* \neq q_{\parallel}$ and $q_{\times}^* \neq q_{\times}$ *a priori*. Therefore the relations (50), (51), (52) and (53) are algebraically exact but are not a rigorous discretization of the conservation laws of mass and momentum. They have to be seen as a first tentative to merge a Boltzmann scheme inside the finite volume framework for a fundamental scheme in two space dimensions.

5 Numerical solid boundary condition

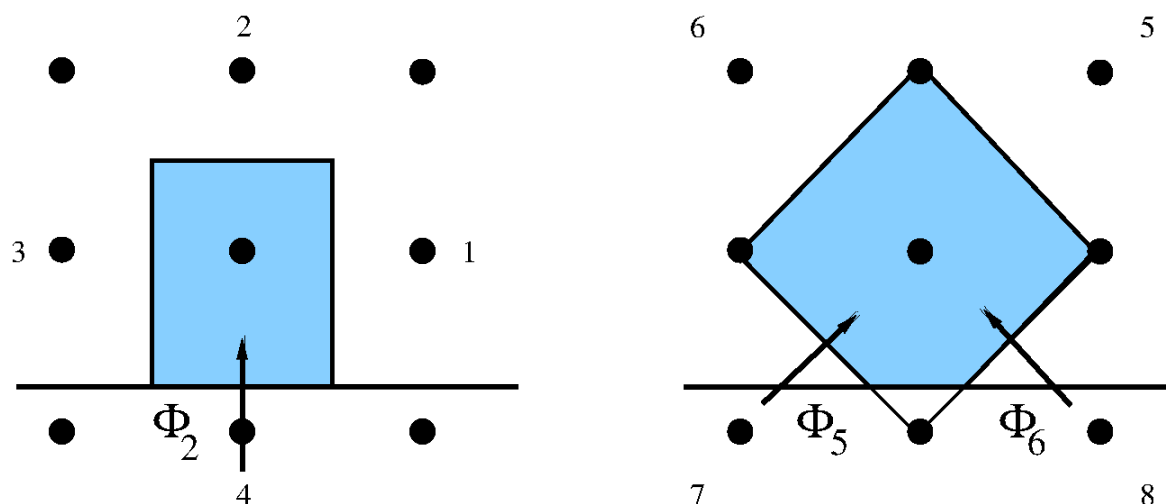


Figure 8. Control finite volumes K_{\parallel} and K_{\times} near the boundary.

- We study in this section the example of an horizontal impenetrable solid boundary for regular geometry that is parallel to the axis of coordinates. We denote by $x \equiv (x_1, x_2)$ a vertex located near the boundary; the latter is in this contribution supposed to be parallel to the x_1 coordinate axis

$$(58) \quad y_w = x_2 - \xi \Delta x.$$

A no-slip boundary condition is supposed to be given for the fluid at the above boundary (58):

$$(59) \quad u(\bullet, y_w) \equiv V(\bullet),$$

where $V(\bullet)$ is some velocity field tangential to the boundary. Then, as illustrated in Figure 8, the number of “post-collision” particles $f_2^*(x - v_2\Delta t)$, $f_5^*(x - v_5\Delta t)$ and $f_6^*(x - v_6\Delta t)$ coming from the neighbours x_4 , x_7 and x_8 respectively of the node x are not given by the general scheme (9).

- We denote by $|K_{\parallel}|$ and $|K_{\times}|$ the measures of the finite volumes around the vertex x defined according to Figure 8. The boundary ∂K_{\parallel} is composed by the four edges a_j for $j = 1$ to 4 and ∂K_{\times} by the **five** edges a_j for $j = 5$ to 9. Note in passing that the edge a_9 is on the solid boundary. Instead of the relations (41) and (42), we have

$$(60) \quad |K_{\parallel}| = \left(\frac{1}{2} + \xi\right) \Delta x^2, \quad |K_{\times}| = (1 + 2\xi - \xi^2) \Delta x^2.$$

$$(61) \quad |a_1| = |a_3| = \left(\frac{1}{2} + \xi\right) \Delta x, \quad |a_2| = |a_4| = \Delta x,$$

$$(62) \quad |a_5| = |a_6| = \Delta x \sqrt{2}, \quad |a_7| = |a_8| = \xi \Delta x \sqrt{2}, \quad |a_9| = 2(1 - \xi) \Delta x.$$

- **Scheme 2. Flux boundary condition for the D2Q9 model.**

We denote by Φ_2 , Φ_5 and Φ_6 the unknown incoming particle numbers. Recall that

$$(63) \quad \Phi_j = f_j^*(x - v_j\Delta t) \equiv f_j^*(x_{\sigma(j)}), \quad j = 2, 5, 6.$$

We use this notation because the vertices x_4 , x_7 and x_8 are *not* defined as nodes of the computational domain. When we write the approximate conservation of mass (50) (51) in the volumes ∂K_{\parallel} and ∂K_{\times} and the conservation of tangential momentum (52) (53) in the control volume ∂K_{\times} , it is possible to define the three unknown particle distributions Φ_2 , Φ_5 , Φ_6 according to

$$(64) \quad \Phi_2 = f_4^* - \frac{1 - 2\xi}{1 + 2\xi} \left(f_2^* - f_4^*(x_2) \right),$$

for the normal input particle number across the boundary and to

$$(65) \quad \Phi_5 = f_8^* + \frac{1 - \xi}{1 + \xi} \left(-f_5^* + f_8^*(x_6) \right) - \frac{1}{\xi(1 + \xi)} \frac{1}{\mathcal{R}_{\Delta}} \frac{\delta q_w}{\lambda}$$

$$(66) \quad \Phi_6 = f_7^* + \frac{1 - \xi}{1 + \xi} \left(-f_6^* + f_7^*(x_5) \right) + \frac{1}{\xi(1 + \xi)} \frac{1}{\mathcal{R}_{\Delta}} \frac{\delta q_w}{\lambda}$$

for the transverse input particle numbers, with \mathcal{R}_Δ and δq_w defined according to

$$(67) \quad \delta q_w = \sum_{j=0}^8 v_j^x f_j(x) - \rho V$$

$$(68) \quad \mathcal{R}_\Delta \equiv \frac{\rho \lambda \Delta x}{\mu}.$$

and λ introduced in (1).

- Note that this kind of truly two-dimensional treatment is unusual in the framework of lattice Boltzmann schemes, except for the pioneering work of [MBG96]. We remark that the incoming particle distributions Φ_2 , Φ_5 , and Φ_6 are expressed as **linear** functions of the other internal particle distributions $f_j^*(x_k)$ and of the boundary data. This is due to the fact that our methodology is essentially based on the conservation laws of mass and momentum that are linear in terms of conserved variables and fluxes. All the nonlinearities are taken in consideration through the collision step $f \rightarrow f^*$.

Construction of Scheme 2.

We first explain the notations used in relations (65) and (66). First, according to the classical form of the Navier Stokes equations [LL59] and to the hypothesis of an impenetrable boundary, the tangential flux τ across the edge a_9 is defined in terms of the viscosity μ and the normal derivative $\frac{\partial u^x}{\partial n}$ of the tangential velocity:

$$(69) \quad \tau = -\mu \frac{\partial u^x}{\partial n}.$$

For the particular case we study in this contribution, the normal n is pointing in the negative y direction. We approximate $-\frac{\partial u^x}{\partial n}$ by a two-point finite difference scheme using the tangential momentum $\sum_{j=0}^8 v_j^x f_j(x)$ and the (supposed to be constant) reference density ρ at the vertex x . Then we have

$$\tau = \mu \frac{u^x(x) - V}{\xi \Delta x} = \frac{\mu}{\rho \xi \Delta x} \left(\sum_{j=0}^8 v_j^x f_j(x) - \rho V \right).$$

It is then natural to consider the difference of tangential momentum δq_w (defined in (67)) between the computed value at the vertex x and the given

value on the (wall) boundary and the grid Reynolds number \mathcal{R}_Δ (defined in (68)) associated with the mesh speed λ and the space increment Δx . With these notations, we have

$$(70) \quad \tau = \frac{\lambda}{\xi \mathcal{R}_\Delta} \delta q_w.$$

• We write now the conservation (50) of partial mass ρ_\parallel . First due to the Boltzmann scheme

$$(71) \quad \rho_\parallel(x, t + \Delta t) - \rho_\parallel^*(x, t) + \sum_{j=1}^3 (f_j^*(x) - f_{\sigma(j)}^*(x_j)) + (f_4^*(x) - \Phi_2) = 0.$$

Second due to the conservation (50) inside the volume K_\parallel :

$$(72) \quad \frac{1}{\Delta t} (\rho_\parallel(x, t + \Delta t) - \rho_\parallel^*(x, t)) + \sum_{j=1}^3 \frac{|a_j|}{|K_\parallel|} \lambda (f_j^*(x) - f_{\sigma(j)}^*(x_j)) = 0,$$

making use of the fact that the mass flux across the boundary a_4 is **null**. We eliminate the quantity $(\rho_\parallel(x, t + \Delta t) - \rho_\parallel^*(x, t))$ between the relations (71) and (72) with the help of the geometrical lemmas (60) and (61). Then the relation (64) is straightforward to derive. We observe that in the “regular” case when $\xi = \frac{1}{2}$, we recover the “bounce-back” boundary condition.

• In a similar way, we write the conservation (51) of partial mass ρ_\times first due to the Boltzmann scheme

$$(73) \quad \left\{ \begin{array}{l} \rho_\times(x, t + \Delta t) - \rho_\times^*(x, t) + \sum_{j=5}^6 (f_j^*(x, t) - f_{\sigma(j)}^*(x_j, t)) + \\ + (f_7^*(x, t) - \Phi_5) + (f_8^*(x, t) - \Phi_6) = 0 \end{array} \right.$$

and second according to the mass conservation (51) inside the volume K_\times :

$$(74) \quad \left\{ \begin{array}{l} \frac{1}{\Delta t} (\rho_\times(x, t + \Delta t) - \rho_\times^*(x, t)) + \\ + \sum_{j=5}^6 \frac{|a_j| \lambda \sqrt{2}}{|K_\times|} (f_j^*(x) - f_{\sigma(j)}^*(x_j)) + \\ + \frac{\lambda \sqrt{2}}{|K_\times|} (|a_7| (f_7^*(x, t) - \Phi_5) + |a_8| (f_8^*(x, t) - \Phi_6)) = 0. \end{array} \right.$$

Once again, the fact that there is no mass flux across the edge a_9 expresses the physical boundary condition. Then by elimination of $(\rho_\times(x, t + \Delta t) - \rho_\times^*(x, t))$ between the relations (73) and (74), we obtain:

$$\begin{aligned} & \sum_{j=5}^6 \left(1 - \frac{|a_j| \lambda \sqrt{2} \Delta t}{|K_\times|}\right) (f_j^*(x) - f_{\sigma(j)}^*(x_j)) \\ & + \left(1 - \frac{|a_7| \lambda \sqrt{2} \Delta t}{|K_\times|}\right) (f_7^*(x) - \Phi_5) + \left(1 - \frac{|a_8| \lambda \sqrt{2} \Delta t}{|K_\times|}\right) (f_8^*(x) - \Phi_6) = 0 \end{aligned}$$

Due to (60) and (62), we have

$$(75) \quad 1 - \frac{|a_5| \lambda \sqrt{2} \Delta t}{|K_\times|} = 1 - \frac{|a_6| \lambda \sqrt{2} \Delta t}{|K_\times|} = -\frac{(1 - \xi)^2}{1 + 2\xi - \xi^2}$$

$$(76) \quad 1 - \frac{|a_7| \lambda \sqrt{2} \Delta t}{|K_\times|} = 1 - \frac{|a_8| \lambda \sqrt{2} \Delta t}{|K_\times|} = \frac{(1 - \xi^2)}{1 + 2\xi - \xi^2}.$$

Then

$$-(1 - \xi) (f_5^* + f_6^* - f_7^*(x_5) - f_8^*(x_6)) + (1 + \xi) (f_7^* - \Phi_5 + f_8^* - \Phi_6) = 0$$

We deduce an expression for the sum $\Phi_5 + \Phi_6$:

$$(77) \quad \Phi_5 + \Phi_6 = f_7^* + f_8^* - \frac{1 - \xi}{1 + \xi} (f_5^* + f_6^* - f_7^*(x_5) - f_8^*(x_6)).$$

• We now carefully express the conservation of tangential momentum. As in the previous cases, we first have the expression directly derived from the scheme (53)

$$(78) \quad \begin{cases} q_\times^x(x, t + \Delta t) - q_\times^{*,x}(x, t) + \sum_{j=5}^6 v_j^x (f_j^*(x) + f_{\sigma(j)}^*(x_j)) + \\ \quad + v_7^x (f_7^*(x, t) + \Phi_5) + v_8^x (f_8^*(x, t) + \Phi_6) = 0 \end{cases}$$

and second we have the (approximate !) conservation (53) of tangential momentum inside the volume K_\times

$$(79) \quad \frac{1}{\Delta t} (q_\times^x(x, t + \Delta t) - q_\times^{*,x}(x, t)) + \frac{1}{|K_\times|} \sum_{j=5}^9 |a_j| \zeta_j^x = 0.$$

Due to (57) and the expressions of tangential speeds for the D2Q9 model, *id est*

$$(80) \quad v_5^x = \lambda, \quad v_6^x = -\lambda, \quad v_7^x = -\lambda, \quad v_8^x = \lambda,$$

we have

$$(81) \quad \begin{cases} \zeta_5^x = \lambda v_5^x \sqrt{2} \left(f_5^* + f_7^*(x_5) \right), & \zeta_6^x = \lambda v_6^x \sqrt{2} \left(f_6^* + f_8^*(x_6) \right), \\ \zeta_7^x = \lambda v_7^x \sqrt{2} \left(f_7^* + \Phi_5 \right), & \zeta_8^x = \lambda v_8^x \sqrt{2} \left(f_8^* + \Phi_6 \right). \end{cases}$$

The last term ζ_9^x corresponds to the stress tensor along the (little) cut edge a_9 which is the fifth edge of control volume K_\times as presented in (62) (see also Figure 8). Then we have simply

$$(82) \quad \zeta_9^x = \tau.$$

We eliminate $(q_\times^x(x, t + \Delta t) - q_\times^{*,x}(x, t))$ between the relations (78) and (79):

$$\begin{aligned} & \sum_{j=5}^6 \left(1 - \frac{|a_j| \lambda \sqrt{2} \Delta t}{|K_\times|} \right) v_j^x \left(f_j^*(x) + f_{\sigma(j)}^*(x_j) \right) + \\ & + \left(1 - \frac{|a_7| \lambda \sqrt{2} \Delta t}{|K_\times|} \right) v_7^x \left(f_7^*(x) + \Phi_5 \right) + \\ & + \left(1 - \frac{|a_8| \lambda \sqrt{2} \Delta t}{|K_\times|} \right) v_8^x \left(f_8^*(x) + \Phi_6 \right) = \frac{|a_9| \Delta t}{|K_\times|} \tau \end{aligned}$$

Due to (60), (75) and (76), we have

$$\begin{aligned} & -(1 - \xi)^2 \left(\lambda \left(f_5^* + f_7^*(x_5) \right) - \lambda \left(f_6^* + f_8^*(x_6) \right) \right) + \\ & + (1 - \xi^2) \left(-\lambda \left(f_7^* + \Phi_5 \right) + \lambda \left(f_8^* + \Phi_6 \right) \right) = 2(1 - \xi) \Delta x \frac{\Delta t}{\Delta x^2} \frac{\lambda}{\xi \mathcal{R}_\Delta} \delta q_w. \end{aligned}$$

We divide the previous expression by $\lambda(1 - \xi)$ and we deduce

$$\begin{aligned} (1 + \xi) \left(\Phi_5 - \Phi_6 \right) &= -(1 - \xi) \left(f_5^* - f_6^* + f_7^*(x_5) - f_8^*(x_6) \right) \\ & - (1 + \xi) \left(f_7^* - f_8^* \right) - 2 \frac{\delta q_w}{\lambda \xi \mathcal{R}_\Delta}. \end{aligned}$$

In other terms:

$$(83) \quad \begin{cases} \Phi_5 - \Phi_6 = -f_7^* + f_8^* - \frac{1-\xi}{1+\xi} \left(f_5^* - f_6^* + f_7^*(x_5) - f_8^*(x_6) \right) \\ -\frac{2}{1+\xi} \frac{1}{\xi} \frac{\delta q_w}{\mathcal{R}_\Delta \lambda}. \end{cases}$$

The relations (65) and (66) are obtained from (77) and (83) by the resolution of a two by two linear system. \square

- **Couette test case.**

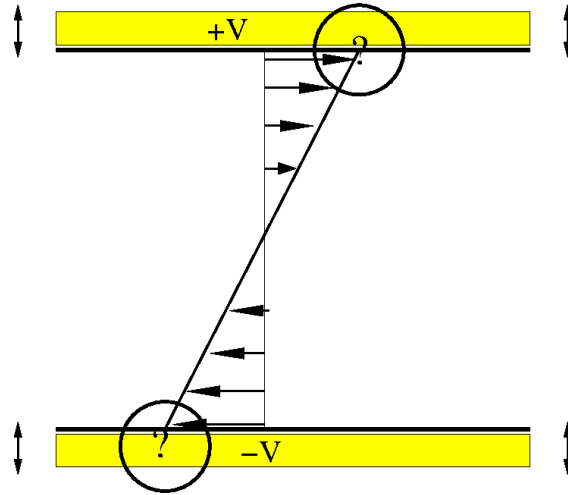


Figure 9. Typical Couette flow.

This classical flow is described in Figure 9. The boundary conditions are simply $+V$ on top and $-V$ at the bottom of a channel. We have used several schemes proposed by D. D’Humières [DH01], Bouzidi *et al* [BFL01], Ginzburg and D’Humières [GH03] for a mesh composed by only 11 mesh points in the direction transverse to the flow. We vary the location of the physical boundary in some proportion ξ relatively to the mesh step Δx . We compute the stationary discrete solution of our lattice Boltzmann scheme. Then with a linear regression fit we measure the location of the point associated with an extrapolated velocity exactly equal to $+V$ or $-V$. Up to seven decimals, all the boundary schemes give the desired result of $+\xi \Delta x$ or $-\xi \Delta x$.

- **Poiseuille test case.**

To test the proposed formulae for boundary conditions, we have also considered the simple Poiseuille flow with two boundaries parallel to the Ox axis located respectively at $y_1 = (1 - \xi)\Delta x$ and $y_2 = (N_y + \xi)\Delta x$ as described in Figure 10. The flow is driven by applying a uniform internal force δf , such that the velocity distribution should be of parabolic form, with null values for y_1 and y_2 and a maximum value $v_m = \delta f(N_y - 1 + 2\xi)^2(\Delta x)^2\rho/(8\mu)$.

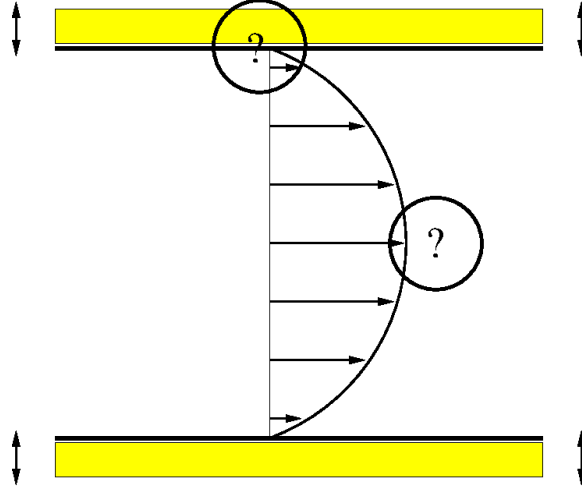


Figure 10. Typical Poiseuille profile and quantities chosen to compare model and theory.

	11 points	21 points	31 points
DH	2.75397×10^{-2}	8.1936×10^{-3}	3.8728×10^{-3}
BFL1	2.5873×10^{-2}	7.6978×10^{-3}	3.6384×10^{-3}
BFL2	7.9811×10^{-3}	2.1898×10^{-3}	1.0049×10^{-3}
IGDH	0	0	0
DL	0	0	0

Table 3. Largest discrepancy of the variation of the maximal velocity for a Poiseuille profile for several boundary schemes and meshes.

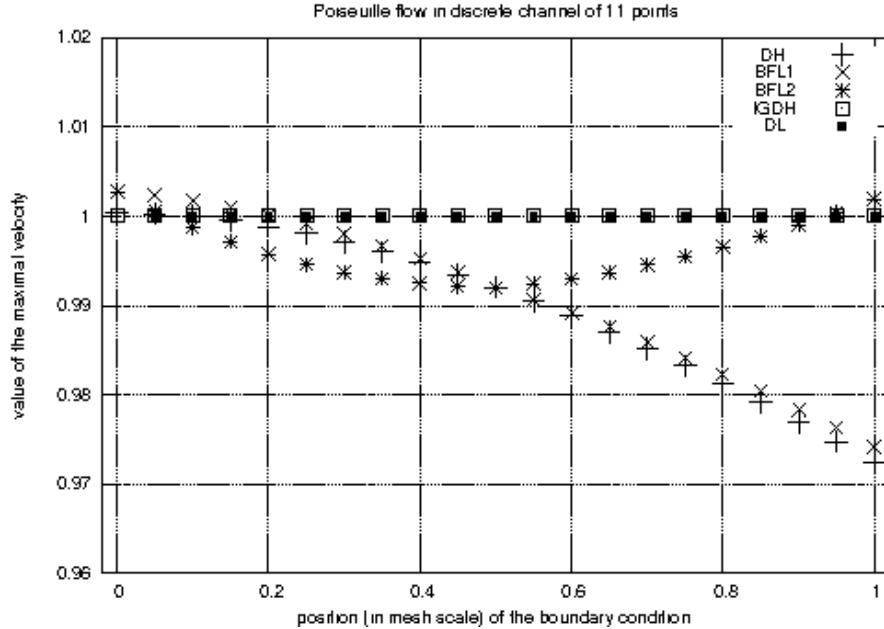


Figure 11 Variation of the maximal velocity for a Poiseuille profile.

- When steady state is reached in the simulation, the velocity profile is fit to a parabolic distribution yielding the maximum velocity and the locations of 0-velocity from which an effective channel width can be deduced. These values are compared to the theoretical values indicated above. Note that when a driving force is applied, we follow [GH03] and perform the parabolic fitting with the quantity $(\sum v_j f_j)/\rho + 1/2\delta f$. Data presented here correspond to the particular case $N_y = 11$. Figure 11 and Table 3 show results for the comparison of the measured maximum velocity normalized by its theoretical value for various boundary schemes. Similarly Figure 12 and Table 4 show the difference between the location of the lower point of 0-velocity and its imposed value *vs* ξ . Obviously the simple bounce-back scheme which gives a constant location leads to an error linear in ξ . For comparison we show the results for a simple boundary condition and indicate that an elaborate scheme, like that of Ginzburg and D’Humières gives the theoretical velocity profile to machine precision. We have also tested whether the proposed scheme satisfies Galilean invariance. This is very well satisfied provided the expression for the equilibrium value of the energy-squared moment includes

a non-linear term $-6\rho(j_x^2 + j_y^2)$ that differ by a factor of 2 from the term provided by the simple BGK equilibrium values [QHL92].

	11 points	21 points	31 points
DH	8.31958×10^{-2}	4.51576×10^{-2}	3.10122×10^{-2}
BFL1	7.81277×10^{-2}	4.24195×10^{-2}	2.91337×10^{-2}
BFL2	2.19920×10^{-2}	1.15029×10^{-2}	7.79×10^{-3}
IGDH	0	0	0
DL	0	0	0

Table 4. Largest discrepancy of the variation of the point of zero velocity for a Poiseuille profile for several boundary schemes and meshes.

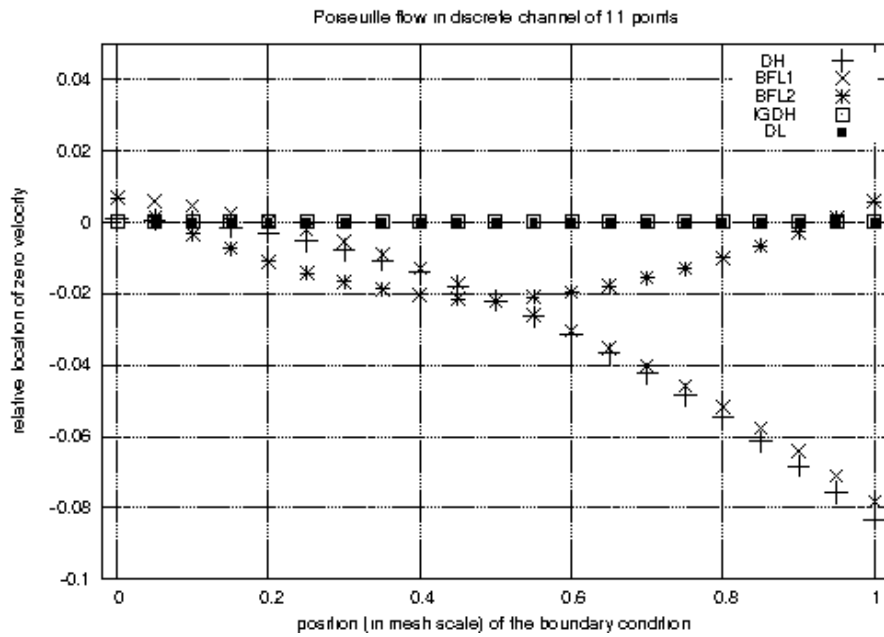


Figure 12 Location of the point of zero velocity for a Poiseuille flow.

- **Stokes eigenmode in a square domain**

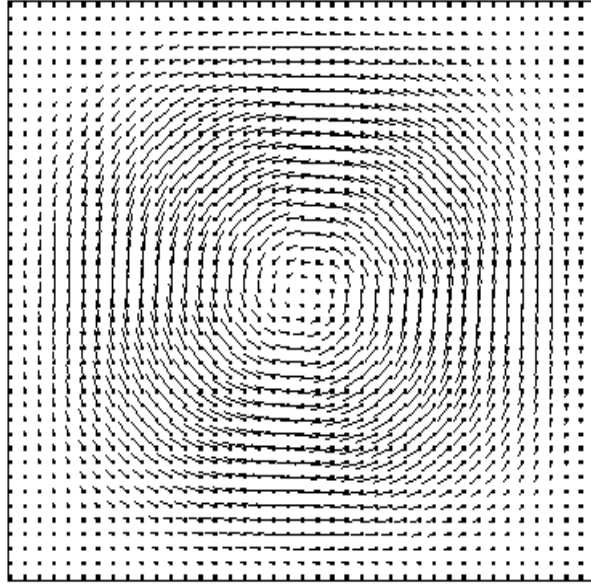


Figure 13. First eigenfunction of the Stokes problem in a square.

To perform a more significant test of the proposed boundary conditions, we considered a simple but very well documented case, that of Stokes modes in a square cavity with homogeneous Dirichlet boundary conditions for velocity [LL04]. Inside the cavity, the fluid follows Stokes equations, for this we use D2Q9 with no non linear term for the equilibrium values of the non-conserved momenta and set the relaxation rates such that there is no fourth order term in the equivalent equations. We use various boundary conditions to obtain zero velocity for the horizontal and vertical boundaries of the square (for $x = 1 - \xi$ and $x = N + \xi$, and $y = 1 - \xi$ and $y = N + \xi$, $0 < \xi < 1$), so that the size of the square is $N - 1 + 2\xi$, with N^2 lattice nodes. The values of the Stokes eigenmodes should scale as

$$(84) \quad \Gamma = \frac{\gamma(j) \nu}{(N - 1 + 2\xi)^2}$$

where ν is the shear viscosity and $\gamma(j)$ depends on the structure of the corresponding eigenmode and is given for small values of j by Labrosse *et al*

[LL04]. We present in Figure 13 the vector field corresponding to the first eigenvalue of the Stokes problem. Using the Arnoldi procedure [Ar51], we determine Γ_{LB} for several values of N and plot in Figure 14 the relative error $\frac{\Gamma_{LB}}{\Gamma} - 1$ vs N^2 for a few ways to implement the boundary conditions. The reader can appreciate the quality of the proposed boundary conditions. The data given in the Figure 14 correspond to the lowest eigenmode, but similar behaviour is observed for higher order modes (up to $j = 30$).

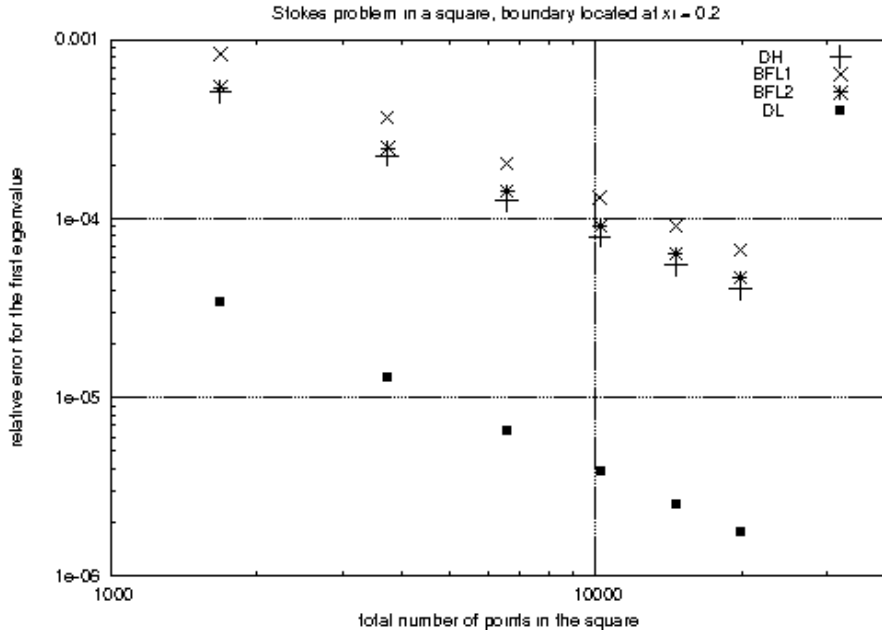


Figure 14. Discrepancies for the first eigenvalue of the Stokes problem with D2Q9 lattice Boltzmann scheme and various boundary conditions.

6 Conclusion

- We have proposed a link between the lattice Boltzmann scheme and the finite volume method. In particular we proposed general relations that define mass and momentum fluxes between two grid points of the lattice Boltzmann scheme. For the D2Q9 model, we have encountered geometrical difficulties and we have proposed the introduction of two families of control volumes in order to define general mass and momentum fluxes. This approach naturally

induces a flux methodology for the treatment of boundary conditions when the boundary flux has naturally a physical meaning. Satisfactory tests for acoustic monodimensional wave, solid two-dimensional boundary for a Couette and Poiseuille flows, eigenmodes for the Stokes problem in a square have been proposed. Our boundary scheme appears to be very precise and can be compared favorably with other high accurate boundary schemes. The next step is to adapt the previous ideas for a geometrically general stable algorithm for two-dimensional boundary conditions. An other extension concerns a more precise treatment of the internal mass and momentum exchanges between the different control volumes. A link with the so-called “reservoir method” [AVCL02] should be explored.

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